X-RAY SPECTROMETRY
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Dispersion corrections to the forward Rayleigh scattering amplitudes around the L-shell of tantalum and lead

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Dispersion corrections to the forward Rayleigh scattering amplitudes of tantalum and lead in the photon energy range 6.4–24.14 keV were determined by a numerical evaluation of the dispersion integral that relates them through the optical theorem to the photoelectric cross-sections. The photoelectric cross-sections were extracted by subtracting the coherent and incoherent scattering contribution from the measured total attenuation cross-section, using a high-resolution, high-purity germanium detector in a narrow-beam good geometry setup. The real part of the dispersion correction to which the relativistic corrections calculated by Kissel and Pratt (S-matrix approach) or Creagh and McAuley (multipole corrections) have been included are in better agreement with the available theoretical values than those values to which the relativistic corrections calculated by Cromer and Liberman (dipole corrections) are added. Copyright © 2006 John Wiley & Sons, Ltd.

INTRODUCTION

It is known from dispersion theory that there exists a relation between the real and imaginary parts f' and f'' of the forward Rayleigh scattering amplitude (also called anomalous scattering factors) and photoelectric cross-section of the element. These relations shown in Eqns (1) and (2) are written based on the optical theorem:[1]

$$f''(E) = \frac{1}{2hcr_0} E\tau \tag{1}$$

where $hc = 1239.84$ MeV fm, $r_0 = 2.8179403 \times 10^{-13}$ cm is the classical electron radius and τ is the photoelectric cross-section of the element[2] at the energy of interest E. The total cross-section σ_{tot}–is given by $\sigma_{tot} = \tau + \sigma_{BBT} - \sigma_{BPP}$, where τ, σ_{BBT} and σ_{BPP} are the photo-effect, photoexcitation and bound pair production cross-sections, respectively. For energies sufficiently away from absorption edge of a particular element, σ_{BBT} and σ_{BPP} are expected to be insignificant for $Z > 10$, below the pair production threshold.[3,4] In the energy region of current interest, if we neglect the spin flip process, the f' and f'' are connected by the modified Kramer's–Kronig transformation, given by

$$f'_R(E) = f'(\infty) - \left(\frac{2}{\pi}\right) P \int_0^\infty \frac{E' f''(E')}{(E^2 - E'^2)} \mathrm{d}E' \tag{2}$$

where P is the Cauchy principal value of the dispersion integral. The second term on the right-hand side represents $f'_{NR}(E)$. It is worth noting that the $f'_{NR}(E)$ values are the non-relativistic values. These values are found to be at variance with the theoretical values by a factor $f'(\infty)$ which is called the high-energy limit or the relativistic correction. It is negative and is generally independent of the energy. $f'(\infty)$ values have been provided by Cromer and Liberman (CL), Creagh and McAuley (CM) and Kissel and Pratt (KP). Among these, the CL corrections are obtained in the dipole approximation; the CM corrections are based on the theoretical treatment that includes multipole approximation in addition to retardation effects.[5] The KP correction calculations are based on the S-matrix approach. The CM and KP corrections are considered to be by far the most accurate. Hence it is possible to determine the dispersion corrections f' and f'' from a set of photoelectric cross-sections using Eqns 1 and 2.

Ever since the first theoretical prediction of x-ray dispersion by Waller,[6] there have been a number of attempts to evaluate the dispersion corrections f' and f''. Based on Waller's[6] theory, for a hydrogen-like atom in a non-relativistic approach, Cromer and Liberman[7] have given extensive tabulations of f' and f'' over a range of wavelengths commonly used by crystallographers. Creagh and McAuley[8] have given tabulations of f' and f''. Kissel and Pratt[9] have tabulated the values of the high-energy limit, based on S-matrix calculations, to be added to f' and also given the values of correction to be added to the Cromer–Liberman f' values. Chantler[10] has provided an extensive tabulation of theoretical form factor, attenuation and scattering data for elements of $Z = 1$–92 from $E = 1$–10 eV to 0.4–1 MeV. Cullen *et al.*[11] have provided a photon data library (EPDL97). This library includes photon interaction data for all elements with atomic number range 1–100 and energy range 1 eV–100 GeV; f' and f' values are also provided. The relativistic correction term used was that calculated by Kissel and Pratt.[9]

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On the experimental side, two types of techniques have mainly been used to determine f' and f''. These are the direct method and the attenuation coefficient method. The direct method is based on (i) the measurement of the refractive index of the specimen of interest, (ii) the determination of the intensities of Bragg reflections[12] and (iii) x-ray interferometery[13] from which f' and f'' values are calculated. The attenuation coefficient method can also be used to obtain the dispersion corrections f' and f''. Sandiago *et al*.,[14] Umesh *et al*.[5] and Appaji Gowda *et al*.[15] have evaluated dispersion corrections around the K-shell for the elements Cu, Ag, Zr, Sn, La, Ce, Pr, Nd, Sm, Gd, Dy, Ho and Er, in the energy range 5–84 keV using the attenuation coefficient method. Drier *et al*.[16] have reported results for Ni, Cu, Zn and Zr around the K-edge and for Ta, W, Pt and Au around the respective L-edges.

In this method, f' and f'' are evaluated by first measuring the total attenuation cross-sections of elements over a wide range in the low-energy x-ray and γ-ray region (below 100 keV). From these data, atomic photoelectric cross-sections are derived by subtracting the relatively insignificant scattering cross-sections. These atomic photoelectric cross-sections are further used to evaluate f' and f''. The evaluation of f' from f'' involves a numerical computation of the dispersion integral (2). Thus, the f'_{NR} values calculated using the photoelectric cross-sections can be used to determine which one of these $f'(\infty)$ values renders a good comparison of $f'_R(E)$ values with the theoretical data.

In this paper, we report $f'_R(E)$ and f' values obtained for Ta and Pb. The $f'_R(E)$ values are calculated by separately adding the relativistic corrections $f'(\infty)$ to the f'_{NR} values. The resulting values are compared with the available theoretical data of Chantler[10] and Cullen *et al*.[11]

EXPERIMENTAL

We measured the total attenuation cross-sections of tantalum and lead in the energy range of interest in a narrow beam, good geometry setup. The detector was a high-resolution hyper-pure germanium detector. The details regarding the experimental setup, method of data acquisition and error analysis along with the calculation of the total attenuation cross-sections are given in an earlier paper.[17]

RESULTS AND DISCUSSION

From the measured total attenuation cross-section values of the tantalum and lead shown in Table 1, the photoelectric cross-sections τ were derived by subtracting the theoretical scattering contribution based on the XCOM values of Berger and Hubbell.[18] Using the corresponding values of the photoelectric cross-section so obtained for energies E both above and below the L-shell, the imaginary part $f'(E)$ of the dispersion correction was calculated using Eqn (1) at each energy E. These values are given in Table 2.

Furthermore, the $f'(E)$ values were used to calculate the $f'_{NR}(E)$ values by a numerical evaluation of the dispersion integral. For this, the lower limit of integration was chosen to be the M_V absorption edge and the upper limit was 1332 keV. Below 6.4 keV up to the M_V edge, photoelectric cross-section data based on XCOM were used since the measurements were made only at and above 6.4 keV in this work. From 6.4 up to 24.14 keV the values given in Table-1 were used. Beyond 24.14 keV, measured values reported earlier were used.[19–22] To evaluate the integral numerically, the energy region was divided into a large number of small intervals. Within each interval (E_i, E_{i+1}), the energy dependence of $f'_i(E)$ was determined by a linear function:

$$f'_i(\mathrm{E}) = (a_i + b_i E) \tag{3}$$

In this interval, the dispersion integral assumes the form

$$I_{i,i+1}(E_s) = \frac{2}{\pi} P \int_{E_i}^{E_{i+1}} \frac{E' f''(E')}{{E_s}^2 - {E'}^2} \mathrm{d}E' \tag{4}$$

Mathematically, the above expression is equivalent to

$$I_{i,i+1}(E_s) = -\frac{2}{\pi}\left[\frac{a_i}{2}\ln\left|\frac{{E_s}^2 - {E_{i+1}}^2}{{E_s}^2 - {E_i}^2}\right| + b_i\left(E_{i+1} - E_i - \frac{E_s}{2}\ln\left|\frac{(E_{i+1}+E_s)}{(E_{i+1}-E_s)}\frac{(E_i - E_s)}{(E_i + E_s)}\right|\right)\right] \tag{5}$$

Using the coefficients a_i and b_i, the dispersion integral was calculated for each interval. The integrals $I_{s-1,s}$ and $I_{s,s+1}$ which are not defined are replaced at once by the integral $I_{s-1,s+1}$. Here, E_{s-1} and E_{s+1} are energies very close to the energy of interest E_s. The final value of the dispersion integral is obtained simply by adding all $_{\mathrm{I}i,i+1}$ values. From these f'_{NR} values, the relativistic correction $f'(\infty)$ suggested by different authors, Cromer and Liberman[7] (dipole correction),

Table 1. Photoelectric cross-sections in barn/atom (errors are to the extent of 3%[17])

	Tantalum		Lead	
Energy (keV)	Present values	XCOM values	Present values	XCOM values
6.4	81 900	84 430	130 368	134 400
8.014	44 650	47 410	75 600	76 350
10.53	58 045	61 100	36 656	37 790
14.4	43 682	43 720	40 750	41 580
24.14	10 692	11 100	17 341	17 600

Table 2. Imaginary part of anomalous scattering factor (f') in e/atom

	Tantalum			Lead		
Energy (keV)	Present values	Chantler values	Cullen values	Present values	Chantler values	Cullen values
6.4	7.50	7.35	7.77	11.94	11.84	12.39
8.041	5.12	5.26	5.47	8.70	8.43	8.77
10.53	8.75	9.14	9.26	5.53	5.50	5.69
14.4	9.00	8.83	8.99	8.40	8.47	8.61
24.14	3.69	3.79	3.83	5.99	6.01	6.09

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Table 3. Relativistic correction $f'(\infty)$ values

Element	CM (multipole correction) 1992	KP (S-matrix correction) 1990	CL (dipole correction) 1970
Tantalum	−0.834	−0.745	−1.385
Lead	−1.116	−0.986	−1.856

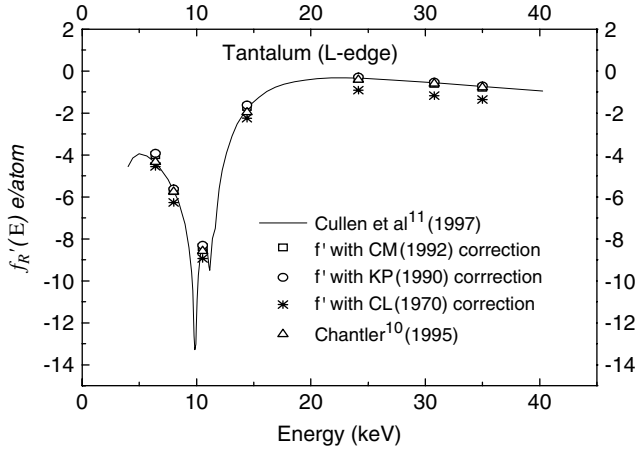

Figure 1. $f'_R(E)$ as a function of energy around the L-edge for tantalum.

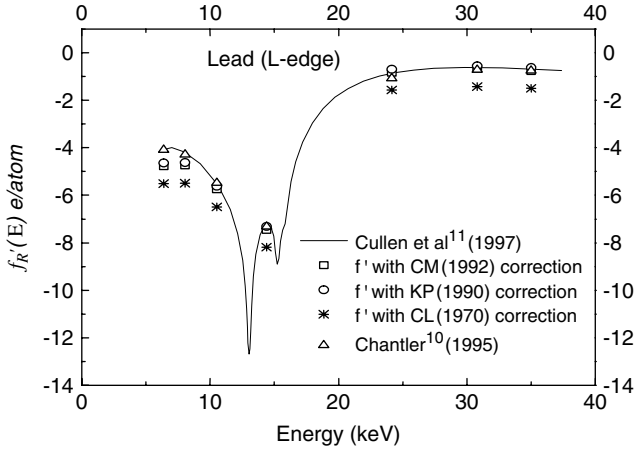

Figure 2. $f'_R(E)$ as a function of energy around the L-edge for lead.

Creagh and McAuley[8] (multipole correction) and Kissel and Pratt[9] (S-matrix correction), for tantalum and lead were separately added and the values of f' were calculated for the elements. The values of $f'(\infty)$ employed are shown in Table 3.

The f'_R values obtained in the case of Ta and Pb are shown in Figs 1 and 2 along with the theoretical data of Cullen *et al*.[11] (KP) and Chantler[10] (CM). It can be seen that the values of $f'_R(E)$ in which CM or KP correction is included follow the trend suggested by theory.

CONCLUSIONS

Based on this study, reasonable values of the dispersion corrections f' and f'' could be obtained from a fairly accurate total attenuation cross-section data set measured in a narrow beam, good geometry setup by employing a high-resolution detector to detect photons emitted by radioisotopes. The present study points to the fact that within the range of experimental errors, the $f'_R(E)$ values in which the $f'(\infty)$ values given by Creagh and McAuley[8] or Kissel and Pratt[9] have been included are in better agreement with the theoretical values of Chantler[10] and Cullen *et al*.[11] than those values to which the relativistic corrections calculated by Cromer and Liberman[7] (dipole corrections)are added. This conclusion also follows from Chantler's paper.[10]

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